What is a “Point Group”? 
Point Group Definition

- A classification scheme for finite objects (molecules)
  - Molecules having the same set of symmetry elements/operations “belong to” the same point group
  - Point groups have labels we will learn
  - We will use the Schoenflies notation (spectroscopy) rather than the Hermann-Mauguin notation (crystallography)
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High symmetry, multiple higher-order \((n > 2)\) rotation axes. Examples: \(T_d, I_h, O_h\)

- Low symmetry, only the identity or that plus only a single mirror plane or an inversion center: \(C_1, C_s, C_i\)
- Linear molecules: \(C_{\infty v}, D_{\infty h}\)
- C groups: \(C_{nv}, C_{nh}, C_n\)
- D groups: \(D_{nd}, D_{nh}, D_n\)
- S groups: \(S_4, S_6, S_8\), etc.; only operations present are based upon \(S_n\)
Types of Point Groups
Labels are the Schoenflies symbols: here are six limiting symmetry types

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The Platonic Solids: Polyhedra with Regular Polygon Faces

Symmetry lowered from the sphere, but still present are multiple higher-order axes.
High Symmetry Groups
These have multiple higher order \((n > 2)\) rotation axes. Example: \(C_{60}\), icosahedral.

Point Group = \(I_h\)
High Symmetry Groups
These have multiple higher order \((n > 2)\) rotation axes. Example: \([\text{B}_{12}\text{H}_{12}]^{2-}\), icosahedral.

Point Group = \(I_h\)

Inorganic Chemistry 5.03
High Symmetry Groups

The tetrahedron has four $C_3$ axes but lacks inversion center.
High Symmetry Groups

The group $T_h$ has four $C_3$ axes (through octahedral faces) and adds the inversion center.
High Symmetry Groups
The group $T$ is a pure rotation group with no mirror planes or inversion centers.
High Symmetry Groups

The group $O_h$ has three $C_4$ axes and an inversion center: $[\text{Mo}_6\text{Cl}_{14}]^{2-}$
High Symmetry Groups
The group $O_h$ has three $C_4$ axes and an inversion center: SF$_6$
Groups of Low Symmetry
The identity alone, or together with one mirror or an inversion center

- The identity only, $C_1$
- The identity plus one mirror plane: $C_s$
- The identity plus an inversion center: $C_i$
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A linear molecule has a $C_\infty$ axis of rotation

- Nitrous oxide, $N_2O$, $N\equiv N\equiv O$, the two ends are different so no $C_2 \perp$ to the $C_\infty$, the point group assignment is $C_{\infty v}$
- Carbon dioxide, $CO_2$, $O\equiv C\equiv O$, the two ends are “symmetry related” and exchangeable by $\perp C_2$ or by $\sigma_h$ so the point group assignment is $D_{\infty h}$
- In general, $D$ groups have $nC_2$ axes $\perp$ to the $C_n$ (single principal rotation axis)
A linear molecule has a $C_\infty$ axis of rotation

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Examples of $C$ groups

A single $C_n$ plus $n$ vertical mirror planes

Point Group = $C_{2v}$
Examples of $C$ groups
A single $C_n$ plus $n$ vertical mirror planes

Point Group = $C_{4v}$
Examples of $C_n$ groups
A single $C_n$ plus a horizontal mirror plane

Point Group = $C_{3h}$
Examples of $C$ groups

A single $C_2$ with no mirror planes: ansa metallocene example of point group $C_2$
Examples of $D$ groups

$D_{nh}$ has $n$ $C_2 \perp$ to the $C_n$, plus a $\sigma_h$.
Examples of $D$ groups

$D_{nh}$ has $n \ C_2 \perp$ to the $C_n$, plus a $\sigma_h$
Examples of $D$ groups

$D_{nd}$ has $n \ C_2 \perp$ to the $C_n$, plus $n\sigma_d$ but no $\sigma_h$; example is $S_4N_4$. 

Point Group = D2d
Examples of $D$ groups

$D_{nd}$ has $n C_2 \perp$ to the $C_n$, plus $n\sigma_d$ but no $\sigma_h$; example is $S_8$.
Examples of $D$ groups

$D_n$ has $n \ C_2 \perp$ to the $C_n$, but no mirror planes; example is $[\text{Fe}((\text{C}_2\text{O}_4)_3)]^{3-}$.
Example of $S_n$ groups

$S_n$ only for $n = 2, 4, 6, \ldots$ but note, $S_2 =\text{inversion}$ so that is $C_i$.
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